NUMERICAL ADVECTION OF CORRELATED TRACERS: PRESERVING MOMENT SEQUENCES DURING TRANSPORT OF AEROSOL MIXTURES

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1. Introduction

Nonlinear transport algorithms designed to reduce numerical diffusion can destroy correlations between moments, isotope abundances, etc. when these scalar densities are transported in models as separate tracers [1, 2]. In case of the particle size/ composition moments of an aerosol, such loss can give rise to unphysical moment sets fatal to aerosol modules based on the quadrature method of moments (QMOM)

In this poster we present a solution to this problem using non-negative least squares (NNLS). In addition to preservation of valid moment sets, the new scheme reduces numerical diffusion during transport and provides greater accuracy for the source apportionment of aerosol mixtures.

The new approach is not limited to moments, it can also be used to improve the accuracy of modal and sectional aerosol simulation methods.

2. Representing aerosols in climate models

(a)
$$\begin{pmatrix} N_1 \\ M_1 \\ N_2 \\ M_2 \\ N_3 \\ \vdots \\ N_k \\ M_k \end{pmatrix}$$
modes or sections, N = number, M = mass

(b)
$$\begin{pmatrix} N_1 \\ \mu_1 \\ \mu_2 \\ \vdots \\ \mu_{i,j,\cdots} \\ N_2 \\ \mu_1 \\ \mu_2 \\ \vdots \\ \mu_{i,j,\cdots} \end{pmatrix}$$
moments including for multiple populations (super-modes)

N = number

μ_k = k^{th} radial or mass moment

$\mu_{i,j}$ = mixed moments (multivariate distributions)

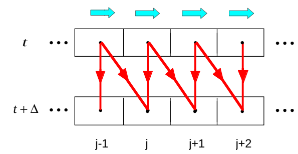
$$\mu_k = \int r^k f(r)dr$$

$$\mu_{i,j} = \int\int m_1^{\,i} m_2^{\,j} f(m_1, m_2, \cdots, m_n) dm_1 \cdots dm_n$$

$m_i =$ mass coordinate of species i

Figure 1. Vector arrays containing sequences of transported scalar densities that can be used to represent aerosols in climate models: (a) modes or sections, (b) moments [3].

3. Correcting advection errors using non-negative least squares (NNLS)



Theorem: A linear combination of valid moment sets with positive coefficients is a valid moment set

Basic idea:

- Assume vectors $\mathbf{v}_j(t)$ contain valid moment sets for all grid cells $\{j\}$ at time t.
- Advect each component as an independent tracer to get intermediate updates $\{\mathbf{v}^{\mathrm{I}}{}_j(t+\Delta)\}$ and un-mix upwind contributions using NNLS:

$$\mathbf{v}^{\mathrm{I}}{}_j(t+\Delta) = c_{j-1}\mathbf{v}_{j-1}(t) + c_j\mathbf{v}_j(t) + error \qquad (c_{j-1}, c_j \geq 0)$$

- Form updated and guaranteed valid vectors as:

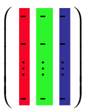
$$\mathbf{v}_j(t+\Delta) = c_{j-1}\mathbf{v}_{j-1}(t) + c_j\mathbf{v}_j(t).$$

4. NNLS for aerosol source apportionment

Same idea as above but with fixed basis vectors containing the valid moments of an initially known distribution of aerosol sources

***Goal:* To decompose the m-vector array of separately advected moments, $\mathbf{b}^{\mathrm{I}}$ which includes any error from transport, into source aerosol vectors R, G, and B.**

Solution:



$$\mathbf{A} \begin{pmatrix} c_R \\ c_G \\ c_B \end{pmatrix} = \mathbf{b}^{\mathrm{I}} + error$$

A c $\mathbf{b}^{\mathrm{I}}$

coefficients c are non-negative with NNLS [4] and the error residual is minimized and dropped to obtain the valid moment array and its source apportionment:

$$\mathbf{b} = \mathbf{c_R v_R} + \mathbf{c_G v_G} + \mathbf{c_B v_B}$$

5. A different kind of advection algorithm test: aerosol source apportionment

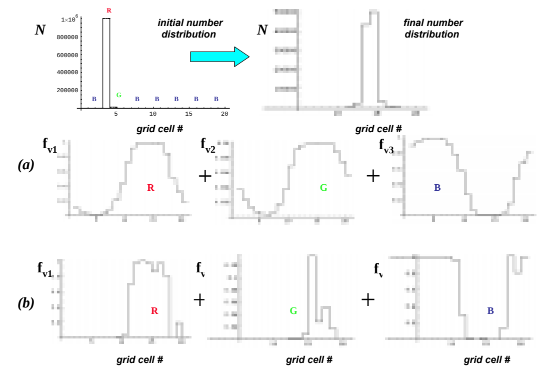


Figure 2. Usual advection tests compare distributions of tracer before and after transport. Top. Initial distribution (left) and final distribution of total particle number after 70 advection steps with a spatially uniform Courant number of 0.15 and a periodic boundary after 20 grid cells (right). Only cell-averaged concentrations are shown. The present test looks at decomposition of transported moments from an aerosol mixture into three component fractions here labeled R, G, and B. The exact final distribution, not shown, is simply the initial distribution translated to the right. Transport was carried out using the quadratic upstream method with flux limitation [5]. (a) Decomposition of final distribution after number vector transport (NVT) with moments 1-3 linked to particle number. (b) NNLS decomposition of the final distribution after separate advection of 4 moments. The new NNLS approach gives a better result and, unlike NVT, doesn't require any modification of the advection algorithm.

Summary

NNLS, which operates independently of the advection routine, insures that only valid moment sets are passed to the aerosol module. Efforts are currently underway to implement NNLS with the BNL aerosol module MATRIX – a highly flexible QMOM platform for use in both regional scale and global climate models

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